21/08/2020

CURRICULUM VITAE ET STUDIORUM: PROF. Maria Cristina Menziani

Personal data:
Present Position: Full Professor in Physical Chemistry
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EDUCATION

- **1983** Degree in Chemistry at the University of Modena
- **1988** Ph. D. in Chemistry at University of Modena
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PREVIOUS POSITIONS AND FELLOSHIPS

- **From October 1987 to October 1988.** PhD Fellowship: Physical Chemistry Laboratory, Oxford University (U.K.)
- **From 1992 to 2002** Researcher of Physical-Chemistry Chemistry Department, Modena University
- **From 2002 to 2016** Associate Professor of Physical Chemistry, Chemistry Department, Modena and Reggio Emilia University**.**

ACADEMIC DUTIES

- Vice-Director of the Department of Chemical and Geological Sciences Unimore 2019-2021
- 2017-2020 Member of "Nucleo di valutazione di Ateneo" UNIMORE
- 2013-2016 Member of "Presidio di Qualità di Ateneo" UNIMORE
- 2007-2010 Member of the National University Council (Area 03-Chemistry)
- 2014- Member of Faculty of the Doctorate Course "Models and Methods for Material and Environmental Sciences" (XXIX)
- 2006-2013 - Director of the School of Graduated Studies "Multiscale Modelling, Computational Simulations and Characterization in Material and Life Sciences"
- 2000 - present Erasmus Coordinator

MEMBERSHIPS AND APPOINTMENTS

- 2020 - 2021President of the Division of Theoretical and Computational Chemistry of the Italian Chemistry Society
- 2017 - 2019 Elected member of the Board of the "Theoretical and Computational Chemistry Division" (Italian Chemical Society)
- 2014-2015 Member of the Scientific Committee of the Italian Chemical Society.
- 2001- 2009, member of the "Centre of Excellence in New Functional Materials, their Design, Diagnostics and Exploitation" Institute of Physics, University of Tartu, Estonia
- 2003 – 2009, Elected member of the Board of the "Physical Chemistry Division" (Italian Chemical Society)
- 2000-2005, Associate Director of the Virtual Centre for rational drug Design (National Foundation for Cancer Research, USA)

VISITS AND STAYS

- **September 1990** Visiting scientist at Physical Chemistry Laboratory, Oxford University (U.K.)
- **June 2002** Visiting scientist at the Institute of Chemistry, University of Tartu (Estonia)
- **May 2013** Visiting scientist at the Interdisciplinary Department on Molecular Systems and Materials of the IRAMIS Institute at the Commissariat à l'énergie atomique et aux énergies alternatives (CEA) in Saclay, France

BRIEF DESCRIPTION OF THE RESEARCH ACTIVITY

My research is aimed at rationalizing and interpreting experimental observed behavior of bio-molecular systems, biomaterials, nanoparticle-biomolecule interactions, by using computational simulation techniques. Many projects are carried out in close collaboration with experimentalists and emphasis on lead/material discovery is given.

- **Domain of competence:**

Computational Spectroscopy
Molecular dynamics (classical & CP), Pametrization
Molecular Simulation Protocols and computational tools for analysis
Protein-ligand and Protein-protein interaction
Homology Modelling, Docking, Drug Design
Quantitative Structure-Activity Relationships

- **Application fields:**

Computational strategies for the study of the structural, dynamics, elastic and spectroscopic properties of crystalline and amorphous inorganic materials, organic molecules and molecular crystals, nanomaterials, interaction between nanoparticle-biological environment, protein-protein, protein-ligand recognition. Development of theoretical molecular descriptors for simple and efficient quantitative structure-properties relationships (QSPR).
List of Publications
http://www.researcherid.com/rid/H-2585-2012
http://orcid.org/0000-0003-3428-5297

FUNDING AND PROJECTS

MAJOR RESEARCH GRANTS:

- **Principal Investigator** FAR2015, *Rational design of curcumin-based bifunctional ligands for early diagnosis and therapy of Alzheimer's disease* (80.000 euro, 18 mesi) Bando UNIMORE su base competitiva.
- **Principal Investigator** del progetto 2010PA3244 *Insight into Silver Nanocube-protein interactions by computational simulations* finanziato con 150.000 core-hours da PRACE Preparatory Access da utilizzarsi sul supercalcolatore Fermi, CINECA, Italy e Marenostrum, BSC, Spain
- **Local Coordinator** PRIN2010-2011, Prot. 2010C4R8M8_002 coordinatore nazionale Prof. A. Agostiano, UniBa, "*Organizzazione Funzionale a Livello Nanoscopico di (Bio)Molecole e Ibridi per Applicazioni nel Campo della Sensoristica, della medicina e delle Biotecnologie".* (88000 euro, 36 mesi)
- **Local Coordinator** Progetto Regionale Emilia Romagna SPINNER 2013 per i dottorati di Ricerca. Titolo del progetto: 'Ottimizzazione delle forme cristalline di farmaci in relazione all'attività, la biodisponibilità, brevettabilità e alla progettazione di polimorfi solvatati e co-cristalli con metodi a basso impatto ambientale'. (45.000, 36 mesi)
- **Local Coordinator** PRIN2008, Prot. 2008J9RNB3 coordinatore nazionale Prof. A. Polimeno, UniPd, "*Time Integration for Molecular Evolution".* (32.180 euro, 24 mesi)

- **Local Coordinator** PRIN 2006, Prot. 2006033728_003, coordinatore nazionale Prof. Delia Picone, UniNa: *Strategie computazionali integrate per l'interpretazione di proprietà strutturali e dinamiche di sistemi nanostrutturali tramite sonde spettroscopicamente attive.* (43.000 euro, 24 mesi)
- **Principal Investigator** Virtual Centre for rational drug Design (National Foundation for Cancer Research, USA) 2000 -2005 ($150,000).

TEACHING ACTIVITIES

- Chimica Computazionale per il corso di Laurea Specialistica/Magistrale in Chimica: A.A. 1996/97 ad oggi.
- Chimica Fisica e Spettroscopia molecolare (Modulo B) per il corso di Laurea Magistrale in Chimica: A.A. 2014/15 ad oggi.
- Chimica Fisica dei Sistemi Naturali per il corso di laure Magistrale in Didattica e Comunicazione delle Scienze: AA 2019/20 ad oggi.
- Chimica dei Sistemi Complessi per il corso di Laurea Magistrale in Chimica: A.A. 2013/2014
- Modellazione Atomistica B con laboratorio per il corso di Laurea Specialistica in Progettazione e sviluppo di nuovi Materiali (Interfacolta' Scienze- Ingegneria): A.A. 2004/2005 al 2009/2010
- Modellazione Atomistica A con laboratorio per il corso di Laurea Specialistica in Progettazione e sviluppo di nuovi Materiali (Interfacolta' Scienze- Ingegneria): da A.A. 2005/2006 al 2006/07
- Informatica Chimica per il corso di Laurea triennale in Chimica: A.A. 2002/2003 al 2009/2010
- Informatica Chimica per il corso di Laurea triennale in Informatica: A.A. 2006/2007 al 2008/2009
- Bioinformatica per il corso di Laurea triennale in Biotecnologie: da A.A. 2002/2003 al 2004/2005.
- Laboratorio di Chimica fisica II (modulo) per il corso di Laurea in Chimica: A.A 2000/2001

Promotor of PhD positions:
XXI Ciclo Marco Campennì (cotutor); Federico Filomia (tutor); XXII Ciclo Nikita Basant (cotutor); Armenio Jorge Moura Barbosa (cotutor); XXIII Ciclo Saxena Puneet (tutor); Damiani Chiara (cotutor); XXV Ciclo DelCadia Marta (tutor); XXVII Ciclo Gambuzzi Elisa (cotutor), Presti Davide (cotutor); XXIX Tavanti Francesco (tutor), Luca Brugnoli (cotutor).

AWARDS

- 2014: Bonino Medal Physical-Chemistry Division of the Italian Chemical Society as a recognition of her researches in the field of Physical-Chemistry.
- Italgas Prize 2001 for Research and Technological Innovation – as a recognition of the research of an international team leaded by Prof. W. Graham Richards.
- Cover page J. Comput. Chem. 2016, issue 37 (DOI: 10.1002/JCC.24340)

ORGANISATION OF SCIENTIFIC MEETINGS AND SCHOOLS

- 2017 Member of the Scientific Committee of the XXVI Congresso Nazionale della Società Chimica Italiana -Paestum.
- 2015 Member of the Scientific Committee of the Workshop "Avogadro Colloquia, Roma, 22 Maggio 2015 https://www.soc.chim.it/it/news/avogadro_colloquia2015
- 2014 Component of the Scientific Committee of the Workshop "Winter Modelling", Modena, 13-14 Marzo 2014
- 2003-2005 Principal Organizer of the "Multiscale Modelling, Computational Simulations and Characterization in Material and Life Sciences School", Modena February 2003, 2004, 2005
- Member of the editorial board of International journal of Molecular Sciences, Section "Molecular Biophysics" ISSN: 1422-0067 (from 2018-)

ACTIVITIES IN REFERRED SCIENTIFIC JOURNALS.

- Referee for European PRACE and ERC proposals. Member of the ERC Advanced Grant Expert Panel (PE4), 2016, 2018. She has taken part to the evaluation exercise for research proposals submitted to the Italian Ministry for Instruction, University and Research (MIUR) within the FIRB-Futuro in Ricerca 2012 and 2013 calls; SIR-Scientific Independence of young Researchers, 2014 call; PRIN- Research projects of national interest, 2012 and 2015 calls. She has also acted as a referee for the 2012 evaluation exercise of Italian Universities and Research Institutes performed by the Italian ANVUR (National Agency for the Evaluation of Universities and Research Institutes).
- Member of high-level review panels for Academy of Finland (Fl) Wellcom Trust (U.K.), Medical Research Council (U.K.), Scuola Normale Superiore di Pisa (It), Agence Nationale de la Recherche (Fr). She acts regularly as referee for many high-impact international journals.

LIST OF SCIENTIFIC PUBLICATIONS ON INTERNATIONAL JOURNALS WITH IF.

http://personale.unimore.it/rubrica/pubblicazioni/menziani